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Structural and elastic DFT study of four structures for Cu_2ZnSnS_4 under high pressure

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Abstract

We have systematically investigated the structural and elastic properties of the zincblende-derived and wurtzite-derived structures of Cu_2ZnSnS_4 (CZTS) under various pressures utilizing first principles calculations within density functional theory (DFT). The results revealed that the enthalpy-pressure curves of kesterite (KS) and stannite (ST) intersect at approximately 32 GPa, while the curves of wurtzite kesterite (WKS) and wurtzite stannite (WST) phases intersect at approximately 52 GPa, which suggests that the phase transitions or mixed crystals occur in the WKS and WST structures. Furthermore, in the KS and ST structures, shear modulus (G) and Young's modulus (E) decrease with an increase in pressure, which indicates that stiffness reduces with increasing pressure. However, in the WKS and WST phases, G and E first decrease and then increase with an increase in pressure. Moreover, owing to Pugh's ductility index (G_H/B_H) being less than 0.57, all four CZTS structures are ductile in nature under different pressures. In the KS and ST phases, Poisson's ratios (γ) increase gradually, when the pressure increases. Whereas, in the WKS and WST structures, the Poisson's ratios (γ) are greater than the Poisson's ratios (γ) under the zero pressure, which indicates better plasticity. Furthermore, it is

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